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Investigation of Two High Temperature Phases of $Ag_4Mn_3O_8$

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Beamline: X7B

Introduction:

Until recently, only the structures of three phases in the system Ag-Mn-O were known. Preparative exploration under an elevated oxygen pressure yielded so far unknown $Ag_4Mn_3O_8$ [1]. Single crystal X-ray investigations have revealed a trigonal crystal system, space group $P3_121$ with lattice parameters *a* = 12,5919(1) and *c* = 15,4978(1) Å. If, in a first step, one represents the MnO_6 octahedra by the central manganese atoms only, a threedimensional framework in R32 pseudosymmetry can be observed. If, in a next step, each group of three manganese atoms in a plane is regarded as a threefold connectivity knot, one obtains the archetypical {10,3} net ($P4_332$), which ideally shows cubic symmetry ($I4_132$)[2, 3]. Thus in $Ag_4Mn_3O_8$ we have encountered a rather unique variety of structural hierarchy [4].

Methods and Materials:

The samples were contained in quartz glass capillaries in a micro reaction cell. X-ray powder diffraction patterns using a MAR345 image plate scanner were collected at various temperatures between 293 and 923 K (Fig. 1). Programs used: FIT2D (data reduction), GUFI (background modeling), ITO (indexing), LeBail-type fits for peak profiles and precise lattice parameters (GSAS and FULLPROF) (Fig. 2).

Results:

In the temperature range from 293 to 923 K we discovered two high temperature phases of $Ag_4Mn_3O_8$. The powder patterns of the phases could be refined showing the space groups predicted in the group-subgroup relationship (Figs. 1, 2). The two high temperature phases of $Ag_4Mn_3O_8$ exist from 473 to 673 K and from 723 to 873 K.

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References

[1] S. Ahlert, K. Friese and M. Jansen, *Z. Anorg. Allg. Chem.* **2002**, 628, 1525-1531.
[2] A. F. Wells, *Acta Crystallogr.* **1954**, 7, 535.
[3] A. F. Wells, *Three-Dimensional Nets and Polyhedra*, John Wiley & Sons, New York, **1977**.
[4] H. G. von Schnering, in: *Jahrbuch Heidelberger Akademie der Wissenschaften*, **1995**.

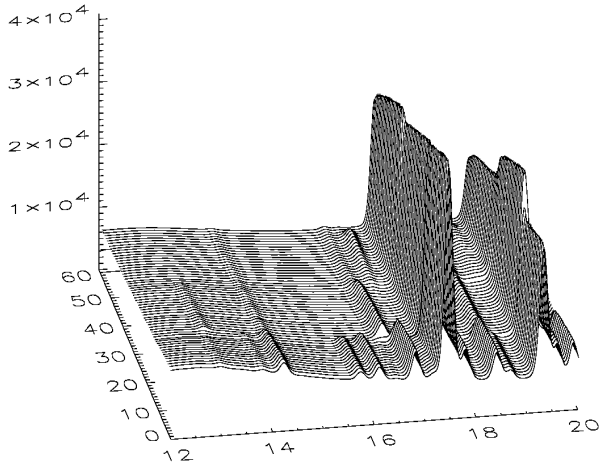

Fig. 1: X-ray powder diffraction patterns of $Ag_4Mn_3O_8$ in dependence of temperature (the temperature difference between consecutive scans is 10K, starting at room temperature) showing two high temperature phase transitions

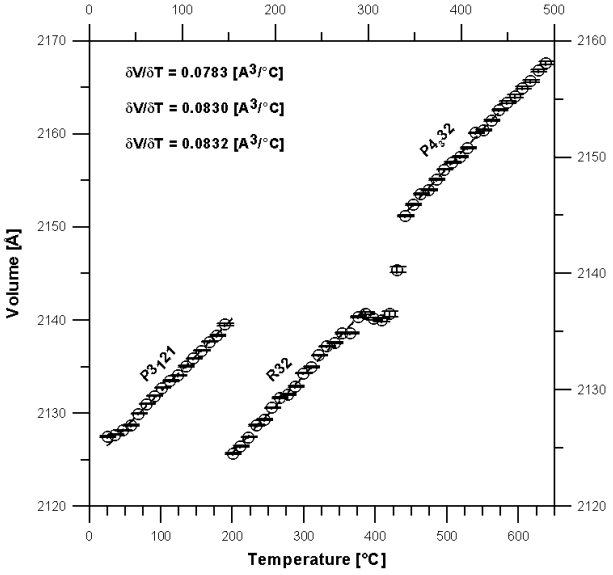

Fig. 2: lattice parameters of $Ag_4Mn_3O_8$ in dependence of temperature.